Supporting Information
The Ideal Gas Thermochemistry of Oxonium Cations

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Table S1 7 term NASA polynomials of oxonium compounds (thermal electron convention) of protonated compounds and radical cations.

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CH3O+  Methylidene Oxonium cation CHOH2+  HF298=1042.05±8. kJ/mol  Burcat G3B3
CHOH2+ Oxonium    T 5/15C  1.H  3.O  1.E -1.G   298.150  6000.000 1000.        1
 4.39380166E+00 7.16728474E-03-2.46127134E-06 3.85124272E-10-2.25476964E-14    2
 1.23503552E+05 3.25046236E-01 1.69308260E+00 1.45930724E-02-9.09655507E-06    3
 1.76040858E-09 5.12383125E-13 1.24252331E+05 1.42806460E+01 1.25329093E+05    4

CH4O*+ Methylene Oxonium cation  CH2OH2*+  HF298=825.9±4.5 kJ/mol Ruscic ATcT 2013
CH2OH2+ Oxonium   T 5/15C  1.H  4.O  1.E -1.G   298.150  6000.000 1000.        1
 5.04696028E+00 8.83268034E-03-2.96312821E-06 4.55893988E-10-2.63627238E-14    2
 9.72441646E+04-1.99964848E+00 1.59132994E+00 2.00143834E-02-1.60986921E-05    3
 6.60975763E-09-7.70735214E-13 9.80978732E+04 1.53918843E+01 9.93323720E+04    4

CH5O+  Methyl Oxonium (Rydberg cation) CH3OH2+  HF298=583.7±8. kJ  Burcat G3B3
CH5O+  CH3OH2+    T11/14C  1.H  5.O  1.E -1.G   298.150  6000.000 1000.        1
 4.12018251E+00 1.23179143E-02-4.21315216E-06 6.57462537E-10-3.84191498E-14    2
 6.81422088E+04 1.71193370E+00 2.63252920E+00 9.23812483E-03 1.43800480E-05    3
-2.22087922E-08 8.80207817E-12 6.89204876E+04 1.11834286E+01 7.02032952E+04    4

C2H5O+ Methyl Methylene Oxonium  CH3-O=CH2+  HF298=676.9±8. kJ  Burcat G3B3
C2H5O+ CH3-O=CH2+ T11/14C  2.H  5.O  1.E -1.G   298.150  6000.000 1000.        1
 5.23682452E+00 1.45674929E-02-5.15192045E-06 8.22867349E-10-4.88896791E-14    2
 7.87093166E+04-3.31148010E+00 3.32715925E+00 7.43454980E-03 2.71006098E-05    3
-3.59610292E-08 1.35250850E-11 7.99157892E+04 9.75450337E+00 8.14129756E+04    4

C2H5O+ Protonated Oxyrane [CH2-CH2]OH+  HF298=715.07±0.62 kJ Ruscic ATcT D 2013
C2H5O+ (CH2CH2)OH+T12/14C  2.H  5.O  1.E -1.G   298.150  6000.000 1000.        1
 5.70791482E+00 1.39321006E-02-4.87755699E-06 7.73937429E-10-4.57782079E-14    2
 8.30274882E+04-8.39211861E+00-5.22964914E-01 2.30971327E-02 5.20358577E-06    3
-2.33955821E-08 1.11084462E-11 8.51270059E+04 2.57116207E+01 8.60026628E+04    4

C2H6O*+ Methyl Methylene Proton Oxonium  CH3-OH-CH2*+  HF298=797.6±8. kJ Burcat
C2H6O+ CH3-OH-CH2+T 5/15C  2.H  6.O  1.E -1.G   298.150  6000.000 1000.        1
 6.85380737E+00 1.52932218E-02-5.29722518E-06 8.34043510E-10-4.90531913E-14    2
 9.27293683E+04-1.05689378E+01 2.50821748E+00 2.11152697E-02 2.81122644E-06    3
-1.66091478E-08 7.80922851E-12 9.42502585E+04 1.34228867E+01 9.59322919E+04    4

C2H7O+  DiMethyl Oxonium  (CH3)2-OH+  HF298=562.24±8. kJ  Burcat G3B3
C2H7O+ (CH3)2OH+  T11/14C  2.H  7.O  1.E -1.G   298.150  6000.000 1000.        1
 5.81266575E+00 1.89420633E-02-6.61986229E-06 1.04878304E-09-6.19569490E-14    2
 6.44582085E+04-7.03041901E+00 3.49195920E+00 9.77638270E-03 3.50079732E-05    3
-4.70880441E-08 1.79334219E-11 6.59209412E+04 8.89898119E+00 6.76213030E+04    4

C2H7O+  Ethyl Oxonium C2H5OH2+  HF298=527.76±8. kJ  Burcat G3B3
C2H7O+ C2H5OH2+   T11/14C  2.H  7.O  1.E -1.G   298.150  6000.000 1000.        1
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 6.18891803E+00 1.79926340E-02-6.24009542E-06 9.83369694E-10-5.78725674E-14    2
 6.03219647E+04-7.85592076E+00 2.86917130E+00 1.73908141E-02 1.49889555E-05    3
-2.77297126E-08 1.13477254E-11 6.17634220E+04 1.17829996E+01 6.34748169E+04    4


C3H7O+ PropyleneOxide Oxonium CH3[CH-CH2]OH+  HF298=648.0±8. kJ  Burcat G3B3
C3H7O+ MeOxoProt  T12/14C  3.H  7.O  1.E -1.G   298.150  6000.000 1000.        1
 8.00791650E+00 1.98766698E-02-7.00852891E-06 1.11739544E-09-6.63134336E-14    2
 7.37876008E+04-1.91729839E+01 1.71414238E-01 3.05635474E-02 6.92713138E-06    3
-2.93671651E-08 1.36322114E-11 7.65168794E+04 2.40418371E+01 7.79360419E+04    4

C3H7O+ CycloTriMethyleneOxide Oxonium [CH2CH2CH2]OH+ HF298=640.85±8. kJ Burcat G3B3
C3H7O+ CyOxonium  T12/14C  3.H  7.O  1.E -1.G   298.150  6000.000 1000.        1
 7.43398460E+00 2.04359385E-02-7.22191223E-06 1.15327670E-09-6.85237610E-14    2
 7.29613893E+04-1.78357142E+01-1.51555883E+00 3.27175286E-02 8.98977573E-06    3
-3.44443374E-08 1.59853557E-11 7.60548693E+04 3.14505091E+01 7.70760995E+04    4

C3H8O*+ Dimethyl Methylene Oxonium  (CH3)2O-CH2*+  HF298=772.8±8. kJ  Burcat G3B3
C3H8O+ (CH3)2O=CH2T10/14C  3.H  8.O  1.E -1.G   298.150  6000.000 1000.        1
 8.67839202E+00 2.17590005E-02-7.63698179E-06 1.21342751E-09-7.18282028E-14    2
 8.86610510E+04-1.98461405E+01 3.64462504E+00 2.27457201E-02 1.85409505E-05    3
-3.57734005E-08 1.47841149E-11 9.07509991E+04 9.46516110E+00 9.29487126E+04    4

C3H9O+  TriMethyl Oxonium (CH3)3O+  HF298=541.716±8. kJ/mol  Burcat G3B3
C3H9O+  (CH3)3O+  T10/14C  3.H  9.O  1.E -1.G   298.150  6000.000 1000.        1
 7.59728406E+00 2.54784347E-02-8.99285110E-06 1.43435890E-09-8.51363342E-14    2
 6.09096282E+04-1.64610245E+01 4.51970904E+00 1.18541575E-02 4.97969882E-05    3
-6.52816266E-08 2.45428621E-11 6.29561255E+04 5.10913040E+00 6.51530878E+04    4

C3H9O+ n-Propanol Protonated Oxonium n-C3H7OH2+  HF298=501.85±8. kJ Burcat G3B3
C3H9O+ nC3H7OH2+  T 5/15C  3.H  9.O  1.E -1.G   298.150  6000.000 1000.        1
 9.44845876E+00 2.35494635E-02-8.48735271E-06 1.36974058E-09-8.18959901E-14    2
 5.54563517E+04-2.49192675E+01 1.57568968E+00 2.98650264E-02 1.75864292E-05    3
-4.05058476E-08 1.72771164E-11 5.84771733E+04 1.97302170E+01 6.03578563E+04    4

C3H9O+ i-Propanol Protonated Oxonium i-C3H7OH2+  HF298=481.8±8. kJ Burcat G3B3
C3H9O+ iC3H7OH2+  T 5/15C  3.H  9.O  1.E -1.G   298.150  6000.000 1000.        1
 9.57409469E+00 2.31713068E-02-8.17316606E-06 1.29960391E-09-7.68969622E-14    2
 5.19914246E+04-2.52943675E+01 2.25481526E+00 3.15666564E-02 9.08108465E-06    3
-3.10362905E-08 1.39286765E-11 5.46444712E+04 1.55201868E+01 5.67452562E+04    4

C4H9O+ TetraHydroFuran Oxonium [CH2CH2CH2CH2]OH+  HF298=529.07±8. kJ Burcat G3B3
C4H9O+ TetHydFuranT12/14C  4.H  9.O  1.E -1.G   298.150  6000.000 1000.        1
 9.27420638E+00 2.68100376E-02-9.51325112E-06 1.52337781E-09-9.06884102E-14    2
 5.83840237E+04-2.82047764E+01-2.08366085E+00 4.20226784E-02 1.12339571E-05    3
-4.29010524E-08 1.97317600E-11 6.23614523E+04 3.45188773E+01 6.36317714E+04    4

C4H11O+ Ethyl DiMethyl Oxonium  C2H5-O-(CH3)2+  HF298=498.±8. kJ  Burcat G3B3
C4H11O+ Oxonium   T10/14C  4.H 11.O  1.E -1.G   298.150  6000.000 1000.        1
 9.41866464E+00 3.13815691E-02-1.11039894E-05 1.77410334E-09-1.05428724E-13    2
 5.46000657E+04-2.53557791E+01 4.76501693E+00 1.78290766E-02 5.63814406E-05    3
-7.68147655E-08 2.92041503E-11 5.73201177E+04 5.46915280E+00 5.98933671E+04    4

C4H11O+ DiEthyl Oxonium  (C2H5)2OH+  HF298=468.08±8. kJ/mol  Burcat G3B3
C4H11O+ (C2H5)2OH+T11/14C  4.H 11.O  1.E -1.G   298.150  6000.000 1000.        1
 9.93034521E+00 3.02853390E-02-1.06660779E-05 1.69877827E-09-1.00731034E-13    2
 5.09606767E+04-2.83500513E+01 3.23373030E+00 3.04473021E-02 2.67898693E-05    3
-4.94050560E-08 2.00818078E-11 5.38304451E+04 1.10075657E+01 5.62964023E+04    4

C5H11O+ PentaHydroxyPyran Oxonium [CH2CH2CH2CH2CH2]OH+ HF298=510.96±8. kJ Burcat
G3B3
C5H11O+ PenHydPyraT 1/15C  5.H 11.O  1.E -1.G   298.150  6000.000 1000.        1
 1.10492507E+01 3.32787293E-02-1.18463934E-05 1.90101634E-09-1.13335364E-13    2
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 5.51041284E+04-3.79392351E+01-2.04330480E+00 4.83518529E-02 1.87019607E-05    3
-5.53878992E-08 2.46466580E-11 5.98475677E+04 3.50599406E+01 6.14548542E+04    4
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C5H13O+ Methyl DiEthyl Oxonium CH_3-O-$(C_2H_5)_2$+ HF298=455.7±8. kJ Burcat G3B3

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C5H13O+ CH3O(C2H5)T11/14C  5.H 13.O  1.E -1.G   298.150  6000.000 1000.        1
 1.23036206E+01 3.57854312E-02-1.26513322E-05 2.02012270E-09-1.19998347E-13    2
 4.82194810E+04-4.14071543E+01 2.26691809E+00 4.31421706E-02 2.28259869E-05    3
-5.39722310E-08 2.30749993E-11 5.21111296E+04 1.56938999E+01 5.48104458E+04    4
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C6H15O+ TriEthyl Oxonium $(C_2H_5)_3O$+ HF298=414.7±8. kJ/mol Burcat G3B3

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C6H15O+ (C2H5)3O+ T11/14C  6.H 15.O  1.E -1.G   298.150  6000.000 1000.        1
 1.38748821E+01 4.23805960E-02-1.50162400E-05 2.40134262E-09-1.42793078E-13    2
 4.23572955E+04-5.00923764E+01 3.65827166E+00 4.63430467E-02 2.98234566E-05    3
-6.17841058E-08 2.54571186E-11 4.65724949E+04 9.09434099E+00 4.98764209E+04    4
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* Oxoniums that are radical cations or distonic ions.